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SDIs in CPlus
NEWS 6 May 27 CPlus super roles and document types searchable in REGISTRY
NEWS 7 Jun 22 STN Patent Forums to be held July 19-22, 2004
NEWS 8 Jun 28 Additional enzyme-catalyzed reactions added to CASREACT
NEWS 9 Jun 28 ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG,
and WATER from CSA now available on STN(R)
NEWS 10 Jul 12 BEILSTEIN enhanced with new display and select options,
resulting in a closer connection to BABS

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:04:41 ON 26 JUL 2004

=> file regis

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:04:59 ON 26 JUL 2004

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 JUL 2004 HIGHEST RN 716315-35-4
DICTIONARY FILE UPDATES: 25 JUL 2004 HIGHEST RN 716315-35-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

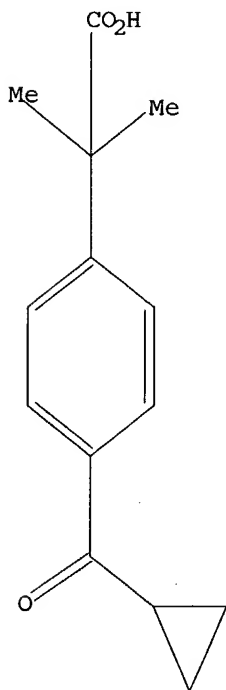
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>
Uploading C:\STNEXP4\QUERIES\10612637.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 11:05:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 157 TO ITERATE

100.0% PROCESSED 157 ITERATIONS

2 ANSWERS

10612637

SEARCH TIME: 00.00.01

L2 2 SEA SSS FUL L1

=> d 1-2 l2

L2 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN

RN 162096-62-0 REGISTRY

CN Cinchonan-9-ol, (8 α ,9R)-, mono[4-(cyclopropylcarbonyl)- α , α -dimethylbenzeneacetate] (salt) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzeneacetic acid, 4-(cyclopropylcarbonyl)- α , α -dimethyl-,
compd. with (8 α ,9R)-cinchonan-9-ol (1:1) (9CI)

FS STEREOSEARCH

MF C19 H22 N2 O . C14 H16 O3

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

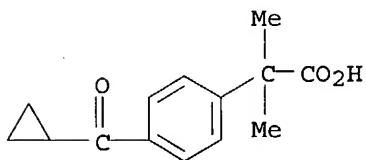
DT.CA CAPLUS document type: Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

CM 1

CRN 162096-54-0

CMF C14 H16 O3

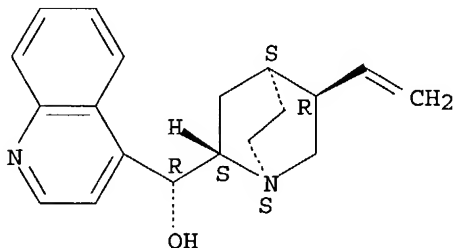


CM 2

CRN 485-71-2

CMF C19 H22 N2 O

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN

RN 162096-54-0 REGISTRY

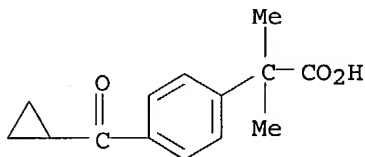
CN Benzeneacetic acid, 4-(cyclopropylcarbonyl)- α , α -dimethyl-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H16 O3

10612637

CI COM
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL
DT.CA CAPLUS document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

159.38

159.59

FILE 'CAPLUS' ENTERED AT 11:06:17 ON 26 JUL 2004

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FILE COVERS 1907 - 26 Jul 2004 VOL 141 ISS 5

FILE LAST UPDATED: 25 Jul 2004 (20040725/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12 full

L3 6 L2

=> d 1-6 bib abs 13

L3 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:5929 CAPLUS

DN 138:73082

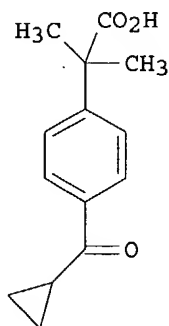
TI Preparation of 4-(cyclopropylcarbonyl)- α,α -dimethylphenylacetic acid

IN Ramesh, Dandala; Umashankar, Das; Divvela, Venkata Naga Srinivasa Rao; Meenakshi, Sunderam Sivakumaran

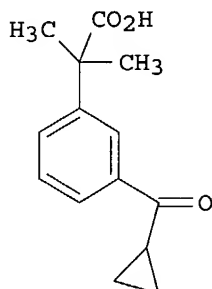
10612637

PA Aurobindo Pharma Limited, India
 SO PCT Int. Appl., 16 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003000658	A1	20030103	WO 2002-IN135	20020619
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW:				
	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	SI 21232	C	20031231	SI 2002-20003	20020619
	EP 1401815	A1	20040331	EP 2002-745778	20020619
	R:				
	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004521942	T2	20040722	JP 2003-507065	20020619
	BG 107476	A	20040130	BG 2003-107476	20030117
	US 2004077900	A1	20040422	US 2003-612637	20030702
PRAI	IN 2001-MA511	A	20010625		
	IN 2001-CH511	A	20010625		
GI	WO 2002-IN135	W	20020619		



I



II

AB A process to obtain highly pure 4-(cyclopropylcarbonyl)-α,α-dimethylphenylacetic acid (I) through crystallization from a mixture of para and meta regioisomers of I and 3-(cyclopropylcarbonyl)-α,α-dimethylphenylacetic acid (II) in cyclohexane, whereby the amount of undesired meta isomer II is decreased to below 0.5%, is described. Compound I is converted in the invention to highly pure terfenadine carboxylate, which is a known antihistaminic (no data).

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

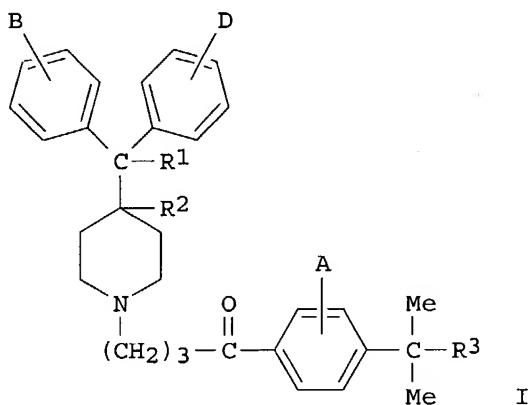
L3 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2002:52000 CAPLUS
 DN 136:102297
 TI Regioselective process for the preparation of 4-[[[(diphenylhydroxymethyl)piperidinyl]butanoyl]-α,α-

NPA

7c

diphenylacetate derivatives as antiallergic agents
IN D'Ambra, Thomas E.
PA USA
SO U.S. Pat. Appl. Publ., 20 pp., Cont. of U.S. Ser. No. 356,172, abandoned.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002007068	A1	20020117	US 2001-758724	20010111
	US 2003018196	A1	20030123	US 2002-235052	20020904
PRAI	US 1999-356172	B1	19990716		
	US 1993-83102	B1	19930624		
	US 1995-382649	A1	19950202		
	US 1997-994357	A1	19971219		
	US 2001-758724	A1	20010111		
OS	CASREACT 136:102297; MARPAT 136:102297				
GI					



AB Substantially pure piperidine derivs. I [wherein R1 = H or OH; R2 = H; or R1 and R2 taken together form a double bond; R3 = CO2H or CO2R4; R4 = alkyl containing 1-6 C atoms; A, B, and D = independently H, halo, alkyl, OH, alkoxy, or other substituents10], useful as antiallergic agents (no data), were prepared. Thus, a mixture of Et 3- and 4-(chloro-1-oxobutyl)- α,α -dimethylphenyl acetate (preparation given) was treated with aqueous NaOH to give a mixture of the 3- and 4-cyclopropyloxomethyl derivs. Regioselective salt formation with cinchonidine, followed by recrystn, gave 4-(cyclopropyloxomethyl)- α,α -dimethylphenylacetic acid. Treatment with Me3SiI afforded 4-(4-iodo-1-oxobutyl)- α,α -dimethylphenylacetic acid, which was esterified with CH2N2 (96%). Coupling with α,α -phenyl-4-piperidinemethanol produced I [R1 = OH; R2 = H; R3 = CO2Me; A, B, and D = H] in 79% yield.

L3 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:408068 CAPLUS
DN 135:19556

TI	Preparation of [(piperidinoalkanoyl)phenyl]propionates and analogs as antihistaminics
IN	Krauss, Richard C.; Strom, Robert M.; Scortichini, Carey L.; Kruper, William J.; Wolf, Richard A.; Wu, Weishi W.; Carr, Albert A.; Hay, David A.; Rudisill, Duane E.; Panzone, Gianbattista

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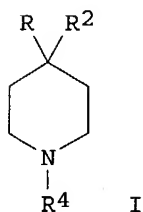
PA Merrell Pharmaceuticals Inc., USA
SO U.S., 60 pp., Cont.-in-part of U.S. Ser. No. 237,466.
CODEN: USXXAM

DT Patent
LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6242606	B1	20010605	US 1994-275685	19940714
	CA 2166059	AA	19950105	CA 1994-2166059	19940526
	CA 2362337	AA	19950105	CA 1994-2362337	19940526
	CA 2362339	AA	19950105	CA 1994-2362339	19940526
	CN 1128987	A	19960814	CN 1994-193031	19940526
	HU 74092	A2	19961128	HU 1995-3705	19940526
	EP 1260504	A1	20021127	EP 2002-12626	19940526
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
	ES 2190442	T3	20030801	ES 1994-919264	19940526
	ZA 9404380	A	19950209	ZA 1994-4380	19940620
	IL 110086	A1	20010913	IL 1994-110086	19940622
	US 6147216	A	20001114	US 1995-458747	19950602
	AU 9915458	A1	19990624	AU 1999-15458	19990208
	AU 734870	B2	20010621		
	CN 1274711	A	20001129	CN 2000-101035	20000112
	US 2001018521	A1	20010830	US 2000-725291	20001129
	US 6566526	B2	20030520		
	US 2001020114	A1	20010906	US 2000-725259	20001129
	US 6552200	B2	20030422		
	US 6340761	B1	20020122	US 2000-725298	20001129
	US 2001000038	A1	20010315	US 2000-726625	20001201
	US 6479663	B2	20021112		
	US 2002198407	A1	20021226	US 2000-726580	20001201
	US 6555689	B2	20030429		
	US 2002007085	A1	20020117	US 2000-729203	20001205
	US 6548675	B2	20030415		
	US 2001021791	A1	20010913	US 2000-731654	20001208
	US 6559312	B2	20030506		
	US 2002077482	A1	20020620	US 2001-818966	20010328
	US 6441179	B2	20020827		
	US 2001031895	A1	20011018	US 2001-824788	20010404
	US 6348597	B2	20020219		
	US 2003220496	A1	20031127	US 2003-364641	20030212
PRAI	US 1993-82693	B2	19930625		
	US 1993-144084	A2	19931027		
	US 1994-237466	A2	19940511		
	AU 1994-70466	A3	19940526		
	CA 1994-2166059	A3	19940526		
	EP 1994-919264	A3	19940526		
	US 1994-275685	A1	19940714		
	US 2000-725259	A3	20001129		
OS	MARPAT 135:19556				
GI					

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AB Title compds. [I; R = R¹CPh₂Om; R¹ = H or OH; R² = H; R¹R² = bond; R⁴ = (CH₂)_nZZ¹CMe₂R³; R³ = CO₂H or alkoxy carbonyl; Z = CO or CH(OH); Z¹ = (2-hydroxy) 1,4-phenylene; m = 0 or 1; N = 1-5] were prepared as antihistaminics (no data). Thus, PhCMe₂CO₂Me was acylated by Cl(CH₂)₃COC₁ and the product aminated by α,α-diphenyl-4-piperidinemethanol to give I.HCl [R = HOCPh₂, R² = H, R⁴ = (CH₂)₃COC₆H₄(CMe₂CO₂Me)-4].

RE.CNT 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:315049 CAPLUS

DN 126:293268

TI Preparation of 4-[4-(4-diphenylmethoxy-1-piperidinyl)-1-oxo(or 1-hydroxy)butyl]-α,α-dimethylphenylacetic acids and its esters as antihistamines, antiallergy agents and bronchodilators

IN D'Ambra, Thomas E.

PA Albany Molecular Research, Inc., USA

SO PCT Int. Appl., 55 pp.

CODEN: PIXXD2

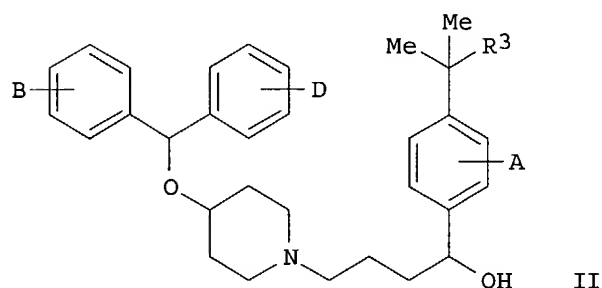
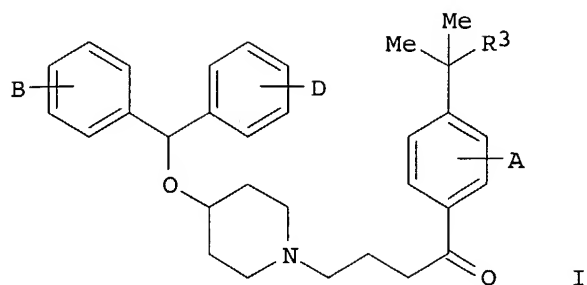
DT Patent

LA English

FAN.CNT 1

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PI	WO 9709983	A1	19970320	WO 1996-US13905	19960830
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	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9671045	A1	19970401	AU 1996-71045	19960830
PRAI	US 1995-527273		19950912		
	WO 1996-US13905		19960830		
OS	CASREACT 126:293268; MARPAT 126:293268				
GI					

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AB The title compds. [I and II; R³ = CO₂H, CO₂C₁₋₆ alkyl; A, B, D = H, halo, alkyl, etc.], useful as antihistamines, antiallergy agents and bronchodilators, were prepared. Thus, reaction of Me 4-(4-chloro-1-oxobutyl)- α,α -dimethylphenylacetate with 4-(diphenylmethoxy)piperidine in the presence of KHCO₃ and KI in PhMe afforded 51% I [R³ = Me; A, B, D = H]. Compds. I are effective at 0.01-20 mg/kg/day.

L3 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:871983 CAPLUS

DN 123:285787

TI Preparation of [(hydroxybenzhydryl)piperidinoalkanoyl]phenylalkanoates and analogs as antihistaminics

IN Krauss, Richard C.; Strom, Robert M.; Scortichini, Carey L.; Kruper, William J.; Wolf, Richard A.; Carr, Albert A.; Rudisill, Duane E.; Panzone, Gianbattista; Hay, David A.; Wu, Weishi W.

PA Merrell Dow Pharmaceuticals Inc., USA

SO PCT Int. Appl., 236 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

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PI	WO 9500480	A1	19950105	WO 1994-US5982	19940526
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	RW:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
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	AU 9470466	A1	19950117	AU 1994-70466	19940526
	AU 699559	B2	19981210		
	EP 705245	A1	19960410	EP 1994-919264	19940526
	EP 705245	B1	20030102		

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HU 74092	A2	19961128	HU 1995-3705	19940526
JP 08512028	T2	19961217	JP 1994-502831	19940526
EP 1260504	A1	20021127	EP 2002-12626	19940526

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE

AT 230395	E	20030115	AT 1994-919264	19940526
ES 2190442	T3	20030801	ES 1994-919264	19940526
ZA 9404380	A	19950209	ZA 1994-4380	19940620
IL 110086	A1	20010913	IL 1994-110086	19940622
FI 9506248	A	19960219	FI 1995-6248	19951222
NO 9505255	A	19960226	NO 1995-5255	19951222
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NO 2002002129	A	19960226	NO 2002-2129	20020503
NO 2003004811	A	19960226	NO 2003-4811	20031028

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US 1994-237466 A 19940511

AU 1994-70466 A3 19940526

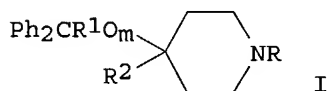
CA 1994-2166059 A3 19940526

EP 1994-919264 A3 19940526

WO 1994-US5982 W 19940526

OS MARPAT 123:285787

GI



AB Title compds. I [R = (CH₂)_nWC₆H₃A(CMe₂R₃)-2,4; A, R₁ = H or OH; R₂ = H; R₁R₂ = bond; R₃ = CO₂H, alkoxycarbonyl, etc.; W = CO, CH(OH); m = 0 or 1; n = 1-5] were prepared as antihistaminics (no data). Thus, PhCMe₂CO₂Et was treated with Cl(CH₂)₃COCl and AlCl₃ and the Ph cyclopropyl ketone product treated with HCl to give 4-[Cl(CH₂)₃CO]C₆H₄CMe₂CO₂Et which was condensed with azacyclonol to give I [R = (CH₂)₃COC₆H₄(CMe₂CO₂Et)-4, R₁ = OH, R₂ = H, m = 0].

L3 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:478306 CAPLUS

DN 122:239548

TI Regioselective preparation of terfenadine analogs.

IN D. Ambra, Thomas E.

PA Albany Molecular Research, Inc., USA

SO PCT Int. Appl., 58 pp.

CODEN: PIXXD2

DT Patent

LA English

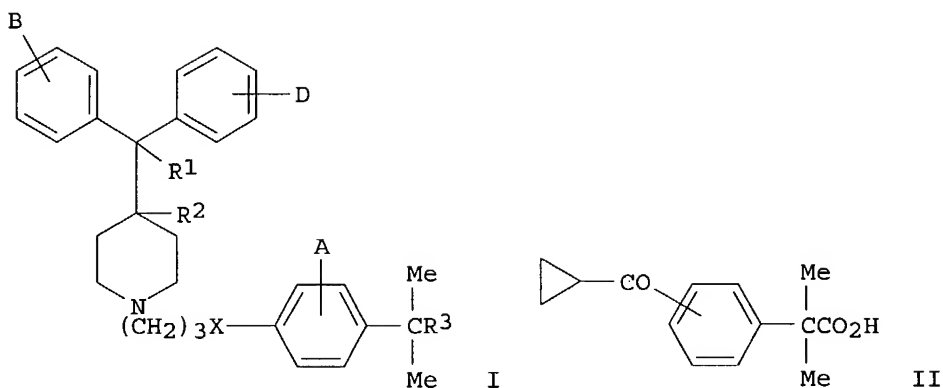
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9500482	A1	19950105	WO 1994-US6873	19940621
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	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
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	JP 3195297	B2	20010806		
	CA 2181089	AA	19941225	CA 1994-2181089	19940621
	CA 2181089	C	20000523		

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CA 2147126	AA	19950105	CA 1994-2147126	19940621
CA 2147126	C	19990824		
CA 2254506	AA	19950105	CA 1994-2254506	19940621
AU 9471748	A1	19950117	AU 1994-71748	19940621
AU 670004	B2	19960627		
EP 703902	A1	19960403	EP 1994-920762	19940621
EP 703902	B1	19981216		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
HU 73235	A2	19960729	HU 1995-3719	19940621
EP 723958	A1	19960731	EP 1996-200338	19940621
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AT 174589	E	19990115	AT 1994-920762	19940621
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OS CASREACT 122:239548; MARPAT 122:239548				
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AB The regioselective preparation of terfenadine analogs I (X = CO, CHOH; R1 = H, OH; R2 = H; R1R2 = bond; R3 = CO2H, CO2R4; R4 = C1-6 alkyl; A, B, D = H, halo, alkyl, OH, alkoxy, etc.) is described. The key steps in the preparation of I were AlCl3-catalyzed acylation of PhCMe2CO2Et with Cl(CH2)3COCl to give a mixture of 3- and 4-Cl(CH2)3COC6H4CMe2CO2Et followed by cyclization-hydrolysis with NaOH to give the 3- and 4-cyclopropylcarbonylphenylacetic acids II which were subsequently separated as their cinchonidine salts.

=> s l3 and purification

297972 PURIFICATION

L4 1 L3 AND PURIFICATION

=> s l3 and crystallization

106875 CRYSTALLIZATION

L5 0 L3 AND CRYSTALLIZATION

=> d 1 bib abs l4

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:5929 CAPLUS

DN 138:73082

TI Preparation of 4-(cyclopropylcarbonyl)- α,α -dimethylphenylacetic acid

IN Ramesh, Dandala; Umashankar, Das; Divvela, Venkata Naga Srinivasa Rao; Meenakshi, Sunderam Sivakumaran

PA Aurobindo Pharma Limited, India

SO PCT Int. Appl., 16 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

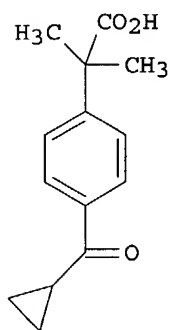
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

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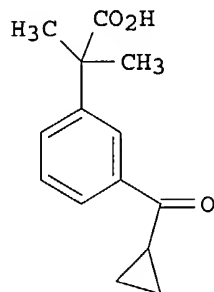
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GI



I



II

AB A process to obtain highly pure 4-(cyclopropylcarbonyl)- α,α -dimethylphenylacetic acid (I) through crystallization from a mixture of para and meta regioisomers of I and 3-(cyclopropylcarbonyl)- α,α -dimethylphenylacetic acid (II) in cyclohexane, whereby the amount of undesired meta isomer II is decreased to below 0.5%, is described. Compound I is converted in the invention to highly pure terfenadine carboxylate, which is a known antihistaminic (no data).

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT